TECHNICAL NOTE R-199

ENERGY TRANSFER THROUGH EVACUATED NONMETALLIC MATERIALS

by D. W. Tarbell

June 1966

RESEARCH LABORATORIES
BROWN ENGINEERING COMPANY, INC.
HUNTSVILLE, ALABAMA

TECHNICAL NOTE R-199

ENERGY TRANSFER THROUGH EVACUATED NONMETALLIC MATERIALS

June 1966

Prepared For

SPACE THERMODYNAMICS BRANCH
RESEARCH PROJECTS LABORATORY
GEORGE C. MARSHALL SPACE FLIGHT CENTER

By

RESEARCH LABORATORIES
BROWN ENGINEERING COMPANY, INC.
HUNTSVILLE, ALABAMA

Contract No. NAS8-20166

Prepared By

D. W. Tarbell

ABSTRACT

Three methods are presented for calculating the spectral absorption coefficient for nonmetallic crystalline solids, and a method for calculating the thermal conductivity of a cubic close-packed array of solid spheres is presented. The three methods in the former are based on a classical, free-ion model, a classical harmonic oscillator model, and a quantum-mechanical harmonic oscillator model. The conductivity calculation is based on the simple addition of conductances in series and parallel.

Approved:

J. E. White, Jr.

J. E. White, Jr.
Research Projects Coordinator

Approved:

R C Watson

R. C. Watson, Jr.
Vice President
Advanced Systems & Technologies

TABLE OF CONTENTS

INTRODUCTION

The task which has been considered during the contract period consisted of the following topics:

- Infrared and microwave interactions
- Heat transfer
- Correlations between thermal and dielectric properties
- Possibilities for determination of temperature and thermal properties of materials by remote sensing of microwave radiation.

Each of the first three topics has been studied. Possibilities for determination of temperature and thermal properties of materials by remote sensing of microwave radiation were not considered. Since most attention has been given to infrared interactions in solids and the problem of conduction of heat through glass spheres, these two topics comprise the bulk of this report. It is mentioned here only that there does exist an equation relating the index of refraction to the electrical conductivity and the absorption coefficient, namely

$$n^2 \kappa = \frac{\mu\sigma}{\nu}$$

where

n - index of refraction,

κ - absorption coefficient,

μ - permeability,

σ - electrical conductivity, and

ν - frequency of the radiation.

There also exists the well-known Wiedemann-Franz law relating the thermal conductivity to the electrical conductivity:

$$\frac{K}{\sigma} = L\,T$$

where

K - thermal conductivity,

σ - electrical conductivity,

T - absolute temperature, and

L - Lorentz number ($= 1.85 \times 10^{-8}$)

These relations can be combined to relate the thermal property, K, to the dielectric property n. However, the above equations are known to be true only for metals and further work was not done on this problem.

DISCUSSION

THE ABSORPTION COEFFICIENT OF CRYSTALLINE SOLIDS

In this section are presented three methods which were used to obtain expressions for the infrared-microwave absorption coefficient of crystalline solids. The first is based on the assumption that the solid is composed of free ions. These ions are assumed to be at rest before the electromagnetic field acts upon them. The second and third methods assume that the ions are in simple harmonic motion before the field is turned on, the former treating the problem classically, the latter, quantum mechanically. Each of the methods assumes that the loss in intensity of an electromagnetic wave as it passes through a solid is proportional to the intensity and to the distance traveled by the beam in the solid. The quantity to be determined is the constant of proportionality, α.

Free Ion Model

This model considers a monochromatic plane-polarized electromagnetic wave incident upon a free ion at rest. The absorption coefficient is found as follows:

$$\alpha \equiv \frac{1}{I} \frac{dI}{dx} \quad . \tag{1}$$

I is the intensity of the beam, i. e., the energy per unit area per unit time passing a given point in the material. dI is the change in intensity as it passes through a thickness of material dx. To calculate α, a distance dx must first be decided upon. In the present case it is natural to assume that this distance is the so-called lattice constant, a, which is the separation of ions in a crystalline solid. Thus,

$$dx = a \quad . \tag{2}$$

The intensity of a plane-polarized monochromatic beam of radiation is given by the well-known expression[1]

$$I = \frac{c\,E_o^2}{8\pi} \tag{3}$$

where c is the velocity of propagation of electromagnetic radiation ($= 3 \times 10^{10}$ cm sec^{-1}) and E_o is the amplitude of the electromagnetic radiation described by

$$E = E_o \sin \omega t$$

where E is the electric field strength, ω is the (angular) frequency of the radiation, and t the time. It therefore remains to calculate dI, the change in intensity.

Considering the area to be the constant value a^2, and the time, Δt, to be the time required for the beam to traverse a unit cell of length a, namely a/c, the problem reduces to a calculation of the work done on a unit charge by the field, i.e., the loss in intensity is given by

$$dI = \frac{W}{a^2 \cdot a/c} = \frac{c\,W}{a^3} \tag{4}$$

where W is the work done on the charge by the field in the time $\Delta t = a/c$. It therefore becomes the problem to calculate W. Now W may be written in the form

$$W = \int_0^{a/c} F \left(\frac{ds}{dt}\right) dt \tag{5}$$

$$F = e\,E = e\,E_o \sin \omega t \tag{6}$$

and (ds/dt) is calculated from Newton's second law as follows:

$$m \frac{d^2 s}{dt^2} = m \frac{dv}{dt} = e\,E_o \sin \omega t \quad .$$

Then

$$v(t) = - \frac{e E_o \cos \omega t}{m\omega} + \frac{e E_o}{m\omega}$$

where the assumption that the particle is initially at rest has been used, i.e., $v(0) = 0$. Substituting this expression and Equation 6 into Equation 5 results in

$$W = \int_0^{a/c} (e E_o \sin \omega t) \left(- \frac{e E_o \cos \omega t}{m\omega} + \frac{e E_o}{m\omega} \right) dt \quad ,$$

which yields upon integration,

$$W = \frac{e^2 E_o^2}{m\omega} \left[- \frac{1}{2\omega} \sin^2 \left(\frac{\omega a}{c} \right) - \frac{1}{\omega} \cos \left(\frac{\omega a}{e} \right) + \frac{1}{\omega} \right] \quad .$$

Now for the infrared-microwave region, the maximum frequency is approximately 10^{15} sec^{-1} and the lattice constant a is typically about[2] 5×10^{-8} cm. Therefore,

$$\frac{\omega a}{c} \lesssim \frac{10^{15} \times 10^{-8}}{10^{10}} = 10^{-3} \quad .$$

The sine and cosine terms can therefore be expanded and only the first order terms kept, so that

$$W = \frac{- e^2 E_o^2 a^2}{2mc^2}$$

This is the expression for the work done on a single ion of mass m. In most ionic crystals there are at least two ions per unit cell. The total work done on both ions is then

$$W = \frac{- e^2 E_o^2 a^2}{2c^2} \left(\frac{1}{m} + \frac{1}{m'} \right) \quad .$$

Inserting this back now into Equation 4 gives

$$dI = \frac{-e^2 E_o^{\ 2}}{2 m c a} \quad .$$

Inserting this and Equations 2 and 3 back into Equation 1 yields

$$\alpha = \frac{4 \pi e^2 (m'+m)}{a^2 c^2 m m'} \quad .$$

This is the final expression for the absorption coefficient. It is seen to be independent of frequency, in contradiction with experiment[3]. However, a short calculation shows that it does yield the correct order of magnitude for a sodium chloride crystal. Using the values

$$e = 4.8 \times 10^{-10} \text{ esu}$$

$$m' = 3.84 \times 10^{-23} \text{ gm (the mass of a Na ion)}$$

$$m = 5.93 \times 10^{-23} \text{ gm (the mass of a Cl ion)}$$

$$a = 5.63 \times 10^{-8} \text{ cm}$$

$$c = 3 \times 10^{10} \text{ cm/sec},$$

α is found to be 0.0435 cm^{-1}. This compares favorably with the AIP Handbook[4] value of 0.02 cm^{-1} for λ=13μ, which is in the middle of the infrared region.

Harmonic Oscillator Model

In order to incorporate frequency into the expression for the absorption coefficient it is now assumed that the ion is a harmonic oscillator. Its displacement from equilibrium can then be written (in the absence of the field)

$$s = \frac{a}{2} \sin \omega_o t \qquad (7)$$

where a is the lattice constant, t is the time and ω_o is the characteristic frequency of the oscillator, given by

$$\omega_o = \left(\frac{k}{m}\right)^{\frac{1}{2}} \tag{8}$$

where k is the force constant characteristic of the crystal and m is the mass of the ion.

The work done on the ion by the field is again given by

$$W = \int_0^{a/c} F \left(\frac{ds}{dt}\right) dt \quad , \tag{9}$$

while the equation for the displacement now becomes

$$m \frac{d^2s}{dt^2} = - k s + e E_o \sin \omega t \quad . \tag{10}$$

The general solution of Equation 10 can be written

$$s(t) = A \sin \omega_o t + B \cos \omega_o t + \frac{\sin \omega t}{\omega_o{}^2 - \omega^2} \left(\frac{e E_o}{m}\right)$$

where A and B are constants to be determined by initial conditions. Using Equation 7 for the initial conditions $s(0) = 0$ and $s'(0) = a \omega_o/2$, gives $B = 0$ and (with some manipulation)

$$A = \frac{a}{2} - \frac{e E_o \omega}{m \omega_o (\omega_o{}^2 - \omega^2)} \quad .$$

Therefore,

$$s(t) = \left[\frac{a}{2} - \frac{e E_o \omega}{m \omega_o (\omega_o{}^2 - \omega^2)}\right] \sin \omega_o t + \left[\frac{e E_o}{m (\omega_o{}^2 - \omega^2)}\right] \sin \omega t \quad ,$$

assuming that $\omega_o^2 \neq \omega^2$. Then

$$\frac{ds}{dt} = A\,\omega_o \cos \omega_o t + C\,\omega \cos \omega t$$

where

$$C \equiv \frac{e\,E_o}{m\,(\omega_o^2-\omega^2)} \quad .$$

Using again Equation 9,

$$W = \int_0^{a/c} (e\,E_o \sin \omega t)\,(A\,\omega_o \cos \omega_o t + C\,\omega \cos \omega t)\,dt \quad .$$

Integrating and again using the fact that $\omega a/c << 1$, for one ion

$$W = \frac{e^2\,E_o^2}{2m\,(\omega_o^2-\omega^2)} \left(\frac{\omega a}{c}\right)^2 \quad .$$

For two ions this becomes

$$W = \frac{e^2\,E_o^2}{2\,(\omega_o^2-\omega^2)} \left(\frac{\omega a}{c}\right)^2 \left(\frac{m+m'}{mm}\right) \quad .$$

Using again Equations 1, 2, 3 and 4,

$$\alpha = \frac{4\pi e^2 \omega^2\,(m+m')}{c^2\,a^2\,(\omega_o^2-\omega^2)\,mm'} \qquad (\omega_o^2 \neq \omega^2) \quad .$$

The constant

$$\frac{4\pi e^2\,(m+m')}{c^2\,a^2\,mm'}$$

has been calculated in the previous section. The final equation for α, therefore, becomes

$$\alpha = (0.0435\ \mathrm{cm}^{-1})\ \frac{\omega^2}{\omega_o^2 - \omega^2} \quad . \tag{11}$$

This gives the desired frequency dependence for α. To compare this with experiment, a value for ω_o is needed. This is found from Equation 8. Using Kittel's[5] method for finding k, the elastic stiffness constant $c_{12} = 0.127 \times 10^{12}$ dyne/cm^2, and $a = 3 \times 10^{-8}$ cm are used to obtain $k = 0.381 \times 10^4$ dyne/cm. The mass will be the reduced mass $\mu = mm'/(m+m') = 23.3 \times 10^{-24}$ gm. Then $\omega_o^2 = 1.635 \times 10^{26}\ \mathrm{sec}^{-2}$ or $\omega_o = 73.8 \times 10^{15}\ \mathrm{sec}^{-1}$.

An attempt was made to fit the data presented for NaCl in the AIP Handbook to Equation 11. The angular frequencies squared, ω^2, for this data, however, varied from $45.2 \times 10^{26}\ \mathrm{sec}^{-2}$ to $210.5 \times 10^{26}\ \mathrm{sec}^{-2}$. Thus in Equation 11, ω_o^2 is entirely negligible with respect to ω^2 and the frequency dependence effectively drops out. The most probable explanation for this is that the wrong value for the elastic stiffness constant was used. However, the only two other values for c are given by Kittel[6] as 0.486×10^{12} dyne/cm^2 and 0.128×10^{12} dyne/cm^2. The former yields an ω_o which is completely out of the range of frequencies given by the Handbook and the latter is nearly identical to the value used. Thus, unless still another elastic stiffness constant is obtained, this is not the source of the error.

Quantum Mechanical Harmonic Oscillator

To obtain the greatest accuracy in any given physical situation, quantum mechanics must be used. In the case of the harmonic oscillator, the wave functions are well-known so that the calculation of the transition probability is much more straightforward than for other systems. The transition probability for a transition from a quantum state n to a quantum state n' is given by[7]

$$\tau^{-1} = \frac{4\pi^2 e^2 I(\omega)}{m^2 c\, \omega^2} \left| \int \overline{W}_{n'} \left[\exp\left(i \vec{k} \cdot \vec{r}\right)\right] \vec{\epsilon}_{\vec{k}\lambda} \cdot \mathrm{grad}\ W_n\, dv \right|^2 \tag{12}$$

where

e - electronic charge

$I(\omega)$ - intensity* of the incident radiation

m - reduced mass of the system

c - velocity of electromagnetic wave propagation

ω - angular frequency of the incident radiation

W_n - wave function of the nth state

$\overline{W_{n'}}$ - complex conjugate of the wave function of the n'th state

$\vec{k}$ - propagation vector of the incident field

$\vec{r}$ - the displacement vector of the reduced mass referred to some aribtrary origin

$\vec{\epsilon}_{\vec{k}\lambda}$ - polarization vector of the incoming field

v - volume of integration.

In the present case, the system is assumed to be one-dimensional in the y-direction and the incoming wave is assumed to be plane-polarized in this direction, so that $\vec{k} \cdot \vec{r} = 0$, $\vec{\epsilon}_{\vec{k}\lambda} \cdot \text{grad } W_n = d W_n/dy$ and $dv = a^2\, dy$ where a is again the lattice constant. Equation 12 therefore becomes

$$\tau^{-1} = \frac{4\pi^2 e^2 I(\omega) a^2}{m^2 c \omega^2} \left| \int \overline{W_{n'}} \frac{d}{dy} W_n \, dy \right|^2 . \qquad (13)$$

To evaluate this expression, it is necessary to have expressions for $\overline{W_{n'}}$ and W_n. These are obtained as follows: the energy of the oscillator is related to the temperature of the specimen in the following way.

$$E = \frac{1}{2} k T$$

---

*Note that this intensity is not the same as the intensity used in the previous sections. They are related by $I = I(\omega)\, \Delta\omega$ where $\Delta\omega$ is the small frequency range of the incident radiation.

where

k - Boltzmann's constant

T - absolute temperature.

The energy of the oscillator is also given by

$$E = \hbar \omega_o \left(n + \frac{1}{2}\right)$$

where $\hbar = h/2\pi$ is Planck's constant divided by 2π. Equating these two expressions shows that

$$n = \frac{k T - \hbar \omega_o}{2 \hbar \omega_o} \quad .$$

Note that this is an approximate result only, for two reasons: (1) the expression $E = \frac{1}{2} k T$, arising from kinetic theory, is only an approximation for the energy of an oscillator, and (2) the constant ω_o in the second equation is also an approximate result since it is calculated from the approximate expression of Kittel[5], $k \approx \beta a$, where β is the elastic stiffness constant.

This expression does yield an approximate expression for n, however, and it will be interesting to make a sample calculation to obtain an approximate number for the transition probability. For T = 300°K and $\omega_o = 1.28 \times 10^{13}\ \text{sec}^{-1}$

$$n \approx \frac{(1.38 \times 10^{-23}\ \text{joule}/°\text{K})(300°\text{K}) - (1.06 \times 10^{-34}\ \text{joule sec})(1.28 \times 10^{13}\ \text{sec}^{-1})}{2\,(1.06 \times 10^{-34}\ \text{joule sec})\,(1.28 \times 10^{13}\ \text{sec}^{-1})}$$

or $n \approx 1$. Now the wave functions $\overline{W}_{n'}$ and W_n are $\overline{W}_o$ and W_1 and are given by Schiff[8] as

$$\overline{W}_o = N_o H_o(\gamma y) \left[\exp\left(-\frac{1}{2} \gamma^2 y^2\right)\right]$$

and

$$W_1 = N_1 H_1 (\gamma y) \left[\exp \left(- \frac{1}{2} \gamma^2 y^2 \right) \right] \quad ,$$

where

$$N_n \equiv \left(\frac{\gamma}{\pi^{\frac{1}{2}} 2^n n!} \right)^{\frac{1}{2}}$$

$$\gamma = \left(\frac{mk}{\hbar^2} \right)^{\frac{1}{4}}$$

and H_o and H_1 are Hermite polynomials, given by

$$H_o = 1$$

and

$$H_1 = 2 \gamma y \quad .$$

Thus, from Equation 13

$$\tau^{-1} = \frac{4 \pi^2 e^2 I(\omega) a^2 D}{m^2 c \omega^2} \tag{14}$$

where

$$D = \frac{mk}{\pi \hbar^2} \left| \int_{-a/2}^{a/2} (1 - \gamma^2 y^2) \left[\exp (- \gamma^2 y^2) \right] dy \right|^2 \tag{15}$$

Since D is not readily evaluated, it is left in this form.

In this method, the absorption coefficient is calculated as follows: the transition probability is the probability per unit time that an oscillator will make a transition from a state n to the next higher state. The energy change for such a transition is

$$\hbar\omega_o\left[\left(n+\frac{1}{2}\right)-\left(n+1+\frac{1}{2}\right)\right]=\hbar\omega_o \quad .$$

The area and the time are the same as before: $A = a^2$ and $t = a/c$, so that the change in intensity of the beam is given by

$$dI = \frac{\tau^{-1}\hbar\omega_o c}{a^3} \quad .$$

The absorption coefficient is therefore

$$\alpha = \frac{1}{I}\,\frac{\tau^{-1}\hbar\omega_o c}{a^4}$$

where τ^{-1} is given by Equation 14.

THE THERMAL CONDUCTIVITY OF AN ARRAY OF SPHERES IN A CUBIC CLOSE-PACKED STRUCTURE

It is the purpose of this section to present a derivation of an expression for the thermal conductivity of an array of spheres under gravitational loading. Such an array is typified by fine powders composed of tiny spherical beads.

Rayleigh[9] considered this problem for the square array of spheres depicted in Figure 1a. The present work considers the case of many layers of the type shown in Figure 1b.

Figure 1

The latter type is considered to be more representative of the way in which spheres will arrange themselves when poured into a container and shaken.

In considering the problem of the thermal conductivity of close-packed spheres, it is first noted that in the ideal case the true conductivity (i. e., omitting any radiation contribution to the measured conductivity) would be zero since there can be no heat transfer across the point contacts made between perfect spheres. In the present case there is a finite area of contact and therefore conductance from one sphere to another because the spheres are deformed under their own weight and the weight of spheres above them. In any application to spacecraft subjected to zero-g conditions, this factor would not contribute but there would still be an area of contact due to van der Waals forces between ions. Electrostatic forces may also enter into the calculation. Whether or not the heat transfer due to these forces is important relative to the radiation transport through the spheres is not known.

The thermal conductivity of any given material is defined according to the apparatus depicted in cross-section in Figure 2. The dark areas are plates held at the constant temperatures T_1 and T_2, the cross-hatched

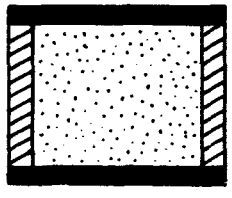

Figure 2

areas are perfect insulators, and the dotted area is the sample whose conductivity is to be measured. Not shown, but also considered to be part of the apparatus, are two perfectly insulating plates at the front and back. In such an apparatus heat is transferred from the plate at the higher temperature to the plate at the lower temperature. The amount of heat per unit time per unit area that is transferred from one plate to the other is proportional to the area of the plates and the difference in temperature, and is inversely proportional to the distance between the plates. This is expressed by the equation

$$Q = K A \frac{(T_1 - T_2)}{\ell} \tag{16}$$

where A is the area of each plate and ℓ is the distance between plates. The constant of proportionality K is known as the thermal conductivity of the sample.

In the present case the sample is a powder composed of tiny glass beads. For ease in visualization, the "two-dimensional" system depicted in cross-section in Figure 3 is first analyzed. The results of this analysis will then be generalized to the case of a three-dimensional close-packed array.

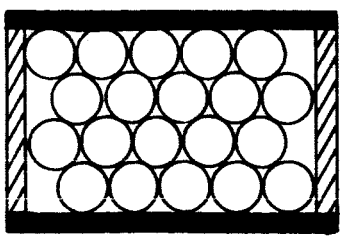

Figure 3

To find K, it is noted that the quantities K and A can be considered together as the conductance, KA, of the array. This total effective conductance can then be found by the usual rules for adding conductances in series and parallel. Since there are a total of 9 contacts between any two given rows, the total conductance between the top row and the second row is $9kA_1$; that between the second and third rows is $9kA_2$, and that between the third and fourth rows is $9kA_3$, where k is the conductivity of the material composing the spheres and the A_i is one of the areas of contact between two spheres in the ith and (i+1)th rows. The total conductance of the array is then given by

$$\frac{1}{KA} = \frac{1}{9kA_1} + \frac{1}{9kA_2} + \frac{1}{9kA_3}$$

$$= \frac{A_2A_3 + A_1A_3 + A_1A_2}{9kA_1A_2A_3}$$

or

$$KA = \frac{9kA_1A_2A_3}{A_2A_3 + A_1A_3 + A_1A_2}$$

Referring again to Figure 3, it is seen that the area A is $(5.5)\pi R^2$ where R is the radius of a sphere. Thus,

$$K = \frac{9kA_1A_2A_3}{(5.5)\pi R\ (A_2A_3 + A_1A_3 + A_1A_2)} \quad . \qquad (17)$$

If one now imagines adding more and more spheres to each row, while keeping the number in one row the same as that in any other row, it is seen that the number of contacts between any two rows will always be (2n-1), where n is the number of spheres in a row. It is also seen that the total area A will be $\left(n + \frac{1}{2}\right)\pi R^2$. Equation 17 can therefore be generalized to

$$K = \frac{(2n-1)kA_1A_2A_3}{\left(n+\frac{1}{2}\right)\pi R^2 (A_2A_3 + A_1A_3 + A_1A_2)} \quad .$$

An examination of Equation 17 further shows that in the case of m rows instead of 4 the equation becomes

$$K = \frac{(2n-1)\, k\, A_1 A_2 A_3 \ldots A_{m-1}}{\left(n+\frac{1}{2}\right)\pi R^2 \left[(A_2 A_3 \ldots A_{m-1}) + (A_1 A_3 A_4 \ldots A_{m-1}) + \ldots + (A_1 A_2 A_3 \ldots A_{m-2})\right]} \tag{18}$$

For an infinite number of beads in each row, this becomes

$$K = \frac{2\, k\, A_1 A_2 A_3 \ldots A_{m-1}}{\pi R^2 \left[(A_2 A_3 \ldots A_{m-1}) + (A_1 A_3 A_4 \ldots A_{m-1}) + \ldots + (A_1 A_2 \ldots A_{m-2})\right]}$$

since the numbers 1 and 1/2 can be neglected. The extension to an infinite number of rows cannot be made at this point.

The extension of the argument to the three-dimensional case is now considered. The system of interest is depicted schematically in Figure 4, adapted from Kittel[2]. The dots represent the centers of the bottom layer of spheres, the circles and crosses the centers of the second and third layers, respectively. (The dashed lines have been put in for ease in visualization; this arrangement is similar to a stack of cannonballs in a park.) The arrangement of Figure 4 is called cubic close-packed as

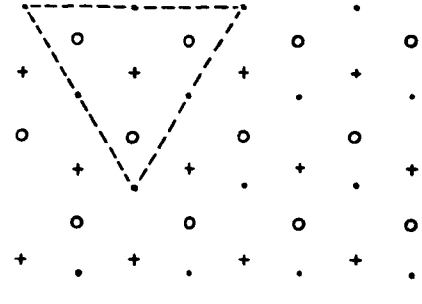

Figure 4

opposed to hexagonal close-packed where the spheres in the third layer lie directly above the spheres in the first layer. The cubic has been chosen over the hexagonal to simplify a later calculation (page 22).

Now the method of adding conductances in the three-dimensional case is no different from that used in the two-dimensional case, i. e., the resultant equation for the conductivity is very similar. Thus, the number of spheres in a row (to be added in parallel) is now the number of spheres in a layer and the number of rows is now the number of layers (to be added in series). It is seen that in this arrangement each sphere is in contact with three below it, instead of two as in the two-dimensional case. In this system there are therefore (3n-x) contacts between any two layers, where n is the number of spheres in a layer and x is a number to take care of end effects*. The total area of the bottom plate in Figure 4 is found from Figure 5. The dimension a is clearly 7R and the dimension b can easily be found by considering the dotted triangle.

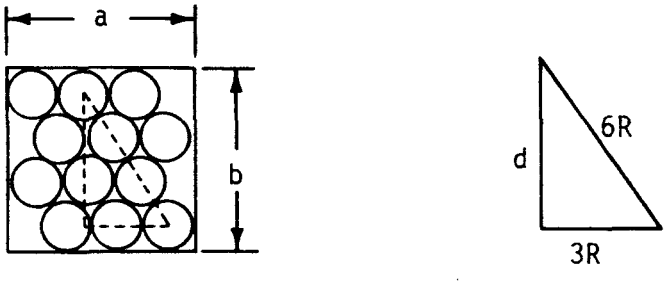

Figure 5

*Contrary to the two-dimensional case, x is variable in the three-dimensional case. For an infinite number of spheres in a layer, there are no end effects however, and x drops out of the expression.

$$d^2 = (6R)^2 - (3R)^2$$

or

$$d = \sqrt{27}\ R$$

$$b = d + 2R$$

$$= (\sqrt{27} + 2)\ R = (3\sqrt{3} + 2)\ R \quad .$$

Thus $A = ab = 7\ (3\sqrt{3} + 2)\ R^2$. Now it can be seen by adding more and more spheres to each row that for p spheres, the dimension a becomes $(2p+1)R$. By adding more and more rows, the dimension b for m rows can be shown to be

$$b = [\sqrt{3}\ (m-1) + 2]\ R \quad .$$

(Note that this expression reduces correctly to 2R when there is only one row: $b = 2R$). The general expression for the area A for p spheres per row and m rows then becomes

$$A = (2p+1)\ [\sqrt{3}\ (m-1)+ 2]\ R^2 \quad .$$

The expression for the conductivity, Equation 18, then becomes

$$K = \frac{(3pm-x)\ k\ A_1\ A_2\ A_3 \ldots A_{r-1}}{(2p+1)\ [\sqrt{3}\ (m-1)+2]\ R^2\ [(A_2A_3 \ldots A_{r-1})+(A_1A_3A_4 \ldots A_{r-1})+ \ldots +(A_1A_2A_3 \ldots A_{r-2})]} \qquad (19)$$

where pm is written for n, the total number of spheres per layer, and r is the number of layers. An expression for the areas A_i is now calculated.

Timoshenko[11] gives for the radius of the circle of the area of contact between two spheres with a force P acting to press them together the following expression:

$$a = \left[\frac{3\pi}{4}\ \frac{P(k_1 + k_2)\ R_1\ R_2}{R_1 + R_2}\right]^{\frac{1}{3}} \qquad (20)$$

where

$k_i = (1-\nu_i^2)/(\pi E_i)$

ν_i - Poisson's ratio

E_i - Young's modulus

R_1 - radius of one sphere

R_2 - radius of the other sphere.

In the case of glass beads assumed to be identical, $k_1 = k_2$ and $R_1 = R_2 \equiv R$, so that Equation 20 reduces to

$$a = \left(\frac{3\pi}{4} PRk\right)^{\frac{1}{3}} \quad . \tag{21}$$

The force between two spheres A and B in the cubic close-packed arrangement is now calculated. Consider Figure 6:

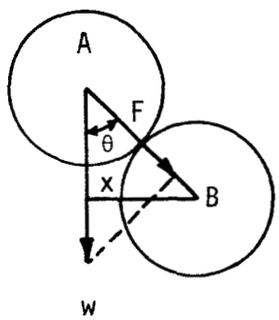

Figure 6

The force F pressing the two beads together is the component of the gravitational force in the direction shown.

$$F = w \cos \theta$$

The angle θ is determined from geometrical considerations:

$$\sin \theta = \frac{x + R}{2R} \quad .$$

To calculate x, consider a top view of the three spheres upon which sphere A rests (Figure 7).

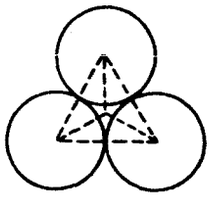

Figure 7

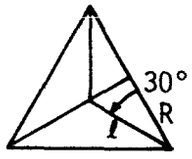

Figure 8

From Figures 6, 7, and 8 it is seen that

$$\ell = x + R$$

or

$$x = \ell - R$$

and from Figure 8 it is clear that

$$\cos 30° = \frac{R}{\ell}$$

or

$$\ell = \frac{R}{\cos 30°}$$

so that

$$\sin\theta = \frac{\frac{R}{\cos 30^\circ} - R + R}{2R}$$

$$= \frac{1}{2\cos 30^\circ} = \frac{1}{\sqrt{3}}$$

$$\cos\theta = \left(\frac{2}{3}\right)^{\frac{1}{2}}$$

and

$$F = w\left(\frac{2}{3}\right)^{\frac{1}{2}} \quad .$$

This is for the case of one bead resting on three beads. For the general case of cubic close-packing, there will be r layers of beads.

An examination of Figure 9 shows that the total force on any given sphere from a given direction is equal to n F where n is the total number of layers above that sphere, and F is the force exerted on it by a single sphere in the layer just above it (Figure 6). The force is transferred directly from one bead to the next in a straight line, so that the force between a sphere in the nth layer and the (n+1)th layer will be given by

$$P_n = n\,w\left(\frac{2}{3}\right)^{\frac{1}{2}} \quad . \tag{22}$$

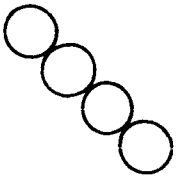

Figure 9

This is the P to be inserted into Equation 21 for the calculation of the area of contact between a bead in the nth layer and one in the (n+1)th layer.

The weight w of a sphere is $\frac{4}{3}\rho\pi R^3$. Inserting this into Equation 22 the force between a sphere in the nth layer and one in the (n+1)th layer is given by

$$P_n = \frac{4}{3} n \rho \pi R^3 \left(\frac{2}{3}\right)^{\frac{1}{2}} \quad .$$

Inserting this and the expression for k (page 20) into Equation 21, the radius of the circle of contact becomes

$$a_n = \left[\frac{3\pi}{4} \cdot \frac{4}{3} n \rho \pi R^3 \left(\frac{2}{3}\right)^{\frac{1}{2}} \frac{R(1-\nu^2)}{\pi E}\right]^{\frac{1}{3}}$$

$$= \left[\frac{n\rho\pi R^4 (1-\nu^2)}{E} \left(\frac{2}{3}\right)^{\frac{1}{2}}\right]^{\frac{1}{3}} \quad .$$

The area then becomes

$$A_n = \pi a_n^2 = \pi \left[\frac{n\rho\pi R^4 (1-\nu^2)}{E} \left(\frac{2}{3}\right)^{\frac{1}{2}}\right]^{\frac{2}{3}} \quad .$$

For identical spheres of a given composition, this equation reduces to

$$A_n = c\, n^{\frac{2}{3}}$$

with

$$c \equiv \pi \left[\frac{\rho\pi R^4 (1-\nu^2)}{E} \left(\frac{2}{3}\right)^{\frac{1}{2}}\right]^{\frac{2}{3}} \quad .$$

Equation 18 for the conductivity then becomes

$$K = \frac{(3pm-x)\, k c \left[(1)^{\frac{2}{3}} (2)^{\frac{2}{3}} (3)^{\frac{2}{3}} \ldots (r-1)^{\frac{2}{3}}\right]}{(2p+1)\left[\sqrt{3}(m-1)+2\right] R^2 \left\{\left[(2)^{\frac{2}{3}} (3)^{\frac{2}{3}} \ldots (r-1)^{\frac{2}{3}}\right] + \left[(1)^{\frac{2}{3}} (3)^{\frac{2}{3}} (4)^{\frac{2}{3}} \ldots (r-1)^{\frac{2}{3}}\right]\right.}$$

$$\left. \frac{(3pm-x) k c \left[(1)^{\frac{2}{3}} (2)^{\frac{2}{3}} (3)^{\frac{2}{3}} \ldots (r-1)^{\frac{2}{3}}\right]}{+ \ldots + \left[(1)^{\frac{2}{3}} (2)^{\frac{2}{3}} (3)^{\frac{2}{3}} \ldots (r-2)^{\frac{2}{3}}\right]} \right\} .$$

Whether or not this expression has a limit as n, p, m, $r \to \infty$ remains to be seen. No answer to this question is immediately obvious.

SUMMARY

Expressions for the absorption coefficient of crystalline solids have been calculated both classically and quantum-mechanically. In the classical calculation the solid was treated first as a collection of free ions and then treated as a collection of harmonic oscillators. While the latter model yielded a frequency-dependent expression, the frequency dependence was found to drop out in making a comparison with experimental data for NaCl using $\omega_o^2 = 1.6 \times 10^{26}$ sec^{-2}. This was because the resonant frequency, ω_o, was negligible compared to the frequencies at which the data were taken. It is strongly suggested by the data that another resonance exists for NaCl near 26μ. This would lead to another force constant and another elastic stiffness constant, not given by Kittel. Since Kittel's book was published in 1957, it is possible that such a resonance has been discussed in the literature. A search of the literature since 1957 is therefore suggested. Data for the absorption coefficient of NaCl in the frequency (squared) range near $\omega_o^2 = 1.6 \times 10^{26}$ sec^{-2} should also be sought. Finally it is noted that the classical equation derived here predicts infinite absorption at the resonant frequency. This could be eliminated by adding a damping term to the equation of motion (Equation 10) and repeating the calculation.

The greatest difficulty in the quantum mechanical treatment is in estimating the quantum numbers of the initial and final states to be inserted in Equation 13 for n and n'. Before evaluating the integral in the expression for D, Equation 15, a more accurate means of determining these quantum numbers should be found. This might be done by considering the energy distribution among the oscillators composing the solid.

In the calculation of the thermal conductivity of an array of close-packed spheres, an expression has been obtained for a finite number of spheres. For a large number of spheres, an evaluation of this expression

would require the use of an electronic computer. Before doing this, however, it should be determined mathematically whether or not the derived expression possesses a limit as the number of spheres becomes large.

REFERENCES

1. Heitler, W., The Quantum Theory of Radiation, Oxford Press, 3rd edition, p. 37, 1954

2. Kittel, C., Introduction to Solid State Physics, John Wiley and Sons, 2nd edition, p. 39, 1956

3. op. cit., p. 114

4. American Institute of Physics Handbook, McGraw-Hill Book Company, Inc., 2nd edition, pp. 6-70, 1963

5. op. cit., Reference 2, p. 113

6. op. cit., Reference 2, p. 93

7. Schiff, L. I., Quantum Mechanics, McGraw-Hill Book Company, Inc., 2nd edition, p. 251, 1955

8. op. cit., p. 61, 64

9. Lord Rayleigh, Phil. Mag. 34, 481 (1892)

10. op. cit., Reference 2, p. 36

11. Timoshenko, S., Theory of Elasticity, McGraw-Hill Book Company, Inc., New York, p. 343, 1934

DOCUMENT CONTROL DATA - R&D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author) Research Laboratories Brown Engineering Company, Inc. Huntsville, Alabama	2a. REPORT SECURITY CLASSIFICATION Unclassified 2b. GROUP N/A

3. REPORT TITLE

"Energy Transfer Through Evacuated Nonmetallic Materials"

4. DESCRIPTIVE NOTES (Type of report and inclusive dates)

Technical Note, June 1966

5. AUTHOR(S) (Last name, first name, initial)

Tarbell, David W.

6. REPORT DATE	7a. TOTAL NO. OF PAGES	7b. NO. OF REFS
June 1966	31	11

8a. CONTRACT OR GRANT NO. NAS8-20166 b. PROJECT NO. N/A c. d.	9a. ORIGINATOR'S REPORT NUMBER(S) TN R-199 9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report) None

10. AVAILABILITY/LIMITATION NOTICES

None

11. SUPPLEMENTARY NOTES None	12. SPONSORING MILITARY ACTIVITY Research Projects Laboratory George C. Marshall Space Flight Center NASA

13. ABSTRACT

Three methods are presented for calculating the spectral absorption coefficient for nonmetallic crystalline solids, and a method for calculating the thermal conductivity of a cubic close-packed array of solid spheres is presented. The three methods in the former are based on a classical, free-ion model, a classical harmonic oscillator model, and a quantum-mechanical harmonic oscillator model. The conductivity is based on the simple addition of conductances in series and parallel.

14. KEY WORDS

spectral absorption coefficient

quantum mechanics

thermal conductivity